Linear Regression

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IIT Gandhinagar

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Linear Regression

- Output is continuous in nature.

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- Examples of linear systems:

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  - $F = ma$

Linear Regression

- Output is continuous in nature.
- Examples of linear systems:
  - $F = ma$
  - $v = u + at$

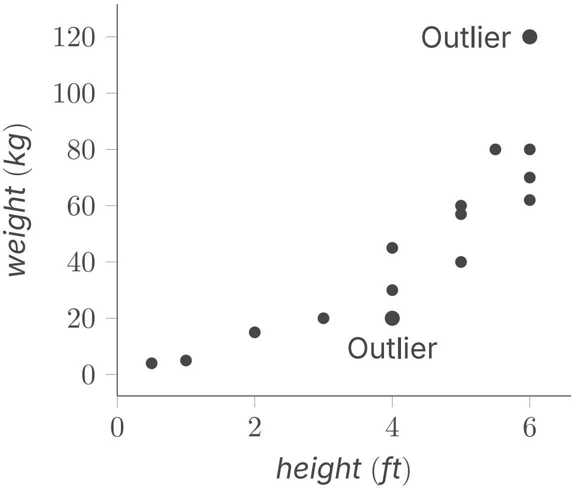
Task at hand

- TASK: Predict Weight = f(height)

Height	Weight
3	29
4	35
5	39
2	20
6	41
7	?
8	?
1	?

The first part of the dataset is the training points. The latter ones are testing points.

Scatter Plot



Matrix representation of the expression

- $\textit{weight}_1 \approx \theta_0 + \theta_1 \cdot \textit{height}_1$

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$$\boxed{\mathit{weight}_i \approx \theta_0 + \theta_1 \cdot \mathit{height}_i}$$

Matrix representation of the expression

$$\begin{bmatrix} \textit{weight}_1 \\ \textit{weight}_2 \\ \dots \\ \textit{weight}_N \end{bmatrix} = \begin{bmatrix} 1 & \textit{height}_1 \\ 1 & \textit{height}_2 \\ \dots & \dots \\ 1 & \textit{height}_N \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

Matrix representation of the expression

$$\begin{bmatrix} weight_1 \\ weight_2 \\ \dots \\ weight_N \end{bmatrix} = \begin{bmatrix} 1 & height_1 \\ 1 & height_2 \\ \dots & \dots \\ 1 & height_N \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

$$\hat{\mathbf{y}}_{n \times 1} = \mathbf{X}_{n \times d} \boldsymbol{\theta}_{d \times 1}$$

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- θ_0 - Bias Term/Intercept Term
- θ_1 - Slope

Extension to multiple dimensions

In the previous example $y = f(x)$, where x is one-dimensional.

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Demand = f(# occupants, Temperature)

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Examples in multiple dimensions.
One example is to predict the water demand of the IITGN campus

Demand = f(# occupants, Temperature)

Demand = Base Demand + K_1 * # occupants + K_2 * Temperature

Intuition

We hope to:

- Learn f: *Demand* = $f(\#occupants, Temperature)$

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- Learn *f*: *Demand* = $f(\#occupants, Temperature)$
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- To predict the condition for the testing set

Linear Relationship

We have

- $x_i = \begin{bmatrix} Temperature_i \\ \#Occupants_i \end{bmatrix}$

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- where $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$
- and $x_i' = \begin{bmatrix} 1 \\ Temperature_i \\ \#Occupants_i \end{bmatrix} = \begin{bmatrix} 1 \\ x_i \end{bmatrix}$
- Notice the transpose in the equation! This is because x_i is a column vector

We can expect the following

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- Demand increases, if # occupants increases, then θ_2 is likely to be positive
- Demand increases, if temperature increases, then θ_1 is likely to be positive
- Base demand is independent of the temperature and the # occupants, but, likely positive, thus θ_0 is likely positive.

Generalized Linear Regression Format

- Assuming N samples for training

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$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix}_{N\times 1} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,M} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,M} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{N,1} & x_{N,2} & \dots & x_{N,M} \end{bmatrix}_{N\times(M+1)} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_M \end{bmatrix}_{(M+1)\times 1}$$

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$$\boxed{\hat{Y} = X\theta}$$

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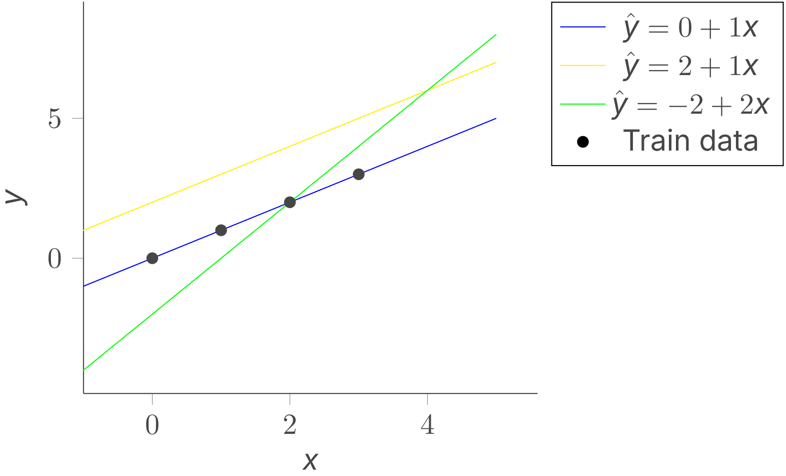
- Let us consider an example in 2d

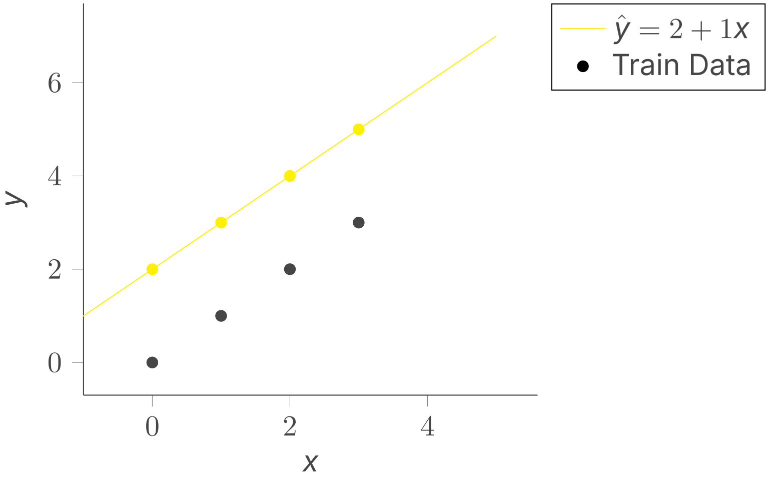
Relationships between feature and target variables

Out of the three fits, which one do we choose?



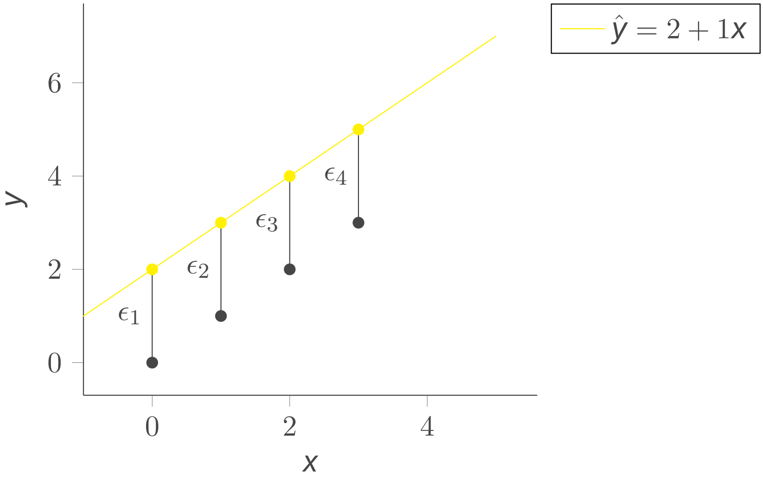
Relationships between feature and target variables

We have $\hat{y} = 2 + 1x$ as one relationship.



Relationships between feature and target variables

How far is our estimated $\hat{y}$ from ground truth y?



Error terms

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- θ_0, θ_1: The parameters of the linear regression
- $\epsilon_i = y_i - \hat{y}_i$
- $\epsilon_i = y_i - (\theta_0 + x_i \cdot \theta_1)$

Good fit

- $|\epsilon_1|$, $|\epsilon_2|$, $|\epsilon_3|$, ... should be small.

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- minimize $\epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_N^2$ - L_2 Norm
- minimize $|\epsilon_1| + |\epsilon_2| + \cdots + |\epsilon_n|$ - L_1 Norm

Normal Equation

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$$Y = X\theta + \epsilon$$

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To Learn: θ

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To Learn: θ
Objective: minimize $\epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_N^2$

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Objective: Minimize $\epsilon^T \epsilon$

Derivation of Normal Equation

$$\boldsymbol{\epsilon} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}$$

$$\boldsymbol{\epsilon}^\top \boldsymbol{\epsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$

$$= \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

This is what we wish to minimize

Minimizing the objective function

$$\frac{\partial \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}}{\partial \boldsymbol{\theta}} = 0$$

- $\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{y}^\top \mathbf{y} = 0$

Substitute the values in the top equation

Minimizing the objective function

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- $\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{y}^\top \mathbf{y} = 0$
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- $\frac{\partial}{\partial \boldsymbol{\theta}} (\boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{\theta}) = 2\mathbf{X}^\top \mathbf{X} \boldsymbol{\theta}$

Substitute the values in the top equation

Normal Equation derivation

$$0 = -2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

$$\mathbf{X}^\top \mathbf{y} = \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta}$$

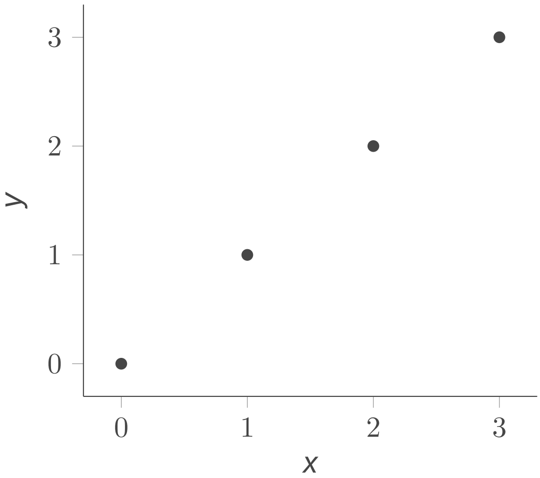
$$\boxed{\hat{\boldsymbol{\theta}}_{OLS} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}}$$

Worked out example

x	y
0	0
1	1
2	2
3	3

Given the data above, find θ_0 and θ_1.

Scatter Plot



Worked out example

$$\mathbf{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}$$

$$\mathbf{X}^\top = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix}$$

$$\mathbf{X}^\top\mathbf{X} = \begin{bmatrix} 4 & 6 \\ 6 & 14 \end{bmatrix}$$

Given the data above, find θ_0 and θ_1.

Worked out example

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{20} \begin{bmatrix} 14 & -6 \\ -6 & 4 \end{bmatrix}$$

$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked out example

$$\theta = (X^T X)^{-1}(X^T y)$$

$$\begin{bmatrix}\theta_0\\ \theta_1\end{bmatrix} = \frac{1}{20}\begin{bmatrix}14 & -6\\ -6 & 4\end{bmatrix}\begin{bmatrix}6\\ 14\end{bmatrix} = \begin{bmatrix}0\\ 1\end{bmatrix}$$

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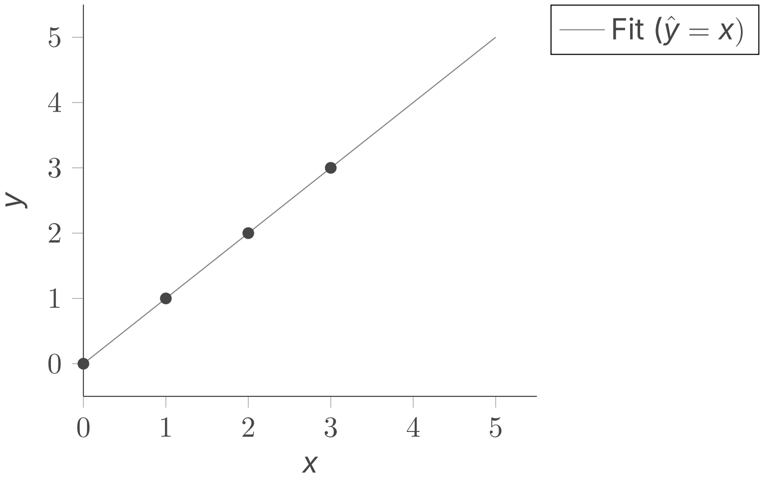
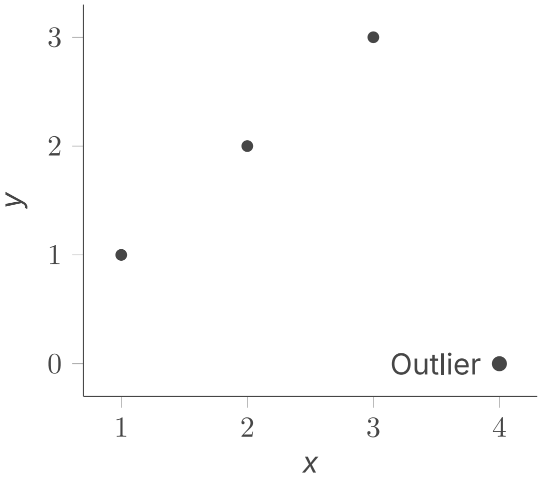


Effect of outlier

x	y
1	1
2	2
3	3
4	0

Compute the θ_0 and θ_1.

Scatter Plot



Worked out example

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}$$

$$X^T = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$X^T X = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

Given the data above, find θ_0 and θ_1.

Worked out example

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{20} \begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}$$

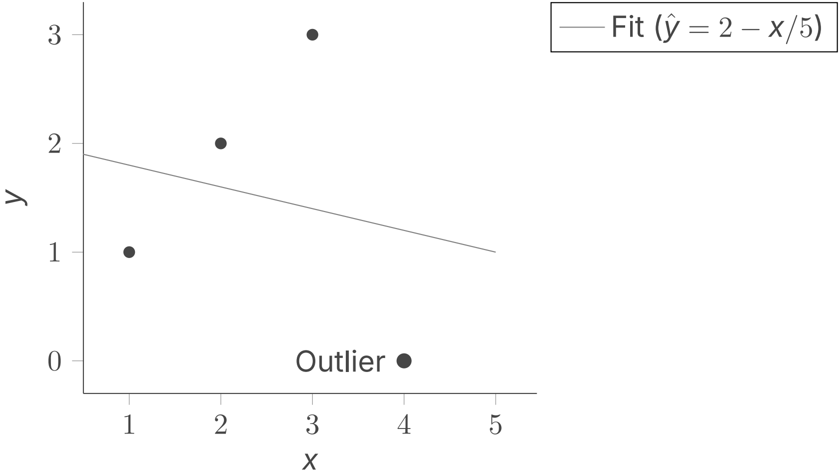
$$\mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Worked out example

$$\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1}(\mathbf{X}^\top \mathbf{y})$$

$$\begin{bmatrix}\theta_0\\ \theta_1\end{bmatrix} = \begin{bmatrix}2\\ (-1/5)\end{bmatrix}$$

Scatter Plot



Variable Transformation

Transform the data, by including the higher power terms in the feature space.

t	s
0	0
1	6
3	24
4	36

The above table represents the data before transformation

Variable Transformation

Add the higher degree features to the previous table

t	t^2	s
0	0	0
1	1	6
3	9	24
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Other transformations: $\log(x), x_1 \times x_2$

A big caveat: Linear in what?![1]

1. $\hat{s} = \theta_0 + \theta_1 * t$ is linear

[1] https://stats.stackexchange.com/questions/8689/what-does-linear-stand-for-in-linear-regression

A big caveat: Linear in what?![1]

1. $\hat{s} = \theta_0 + \theta_1 * t$ is linear
2. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2$ linear?

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3. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2 + \theta_3 * \cos(t^3)$ linear?

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5. All except #4 are linear models!

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2. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2$ linear?
3. Is $\hat{s} = \theta_0 + \theta_1 * t + \theta_2 * t^2 + \theta_3 * \cos(t^3)$ linear?
4. Is $\hat{s} = \theta_0 + \theta_1 * t + e^{\theta_2} * t$ linear?
5. All except #4 are linear models!
6. Linear refers to the relationship between the parameters that you are estimating (θ) and the outcome

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- We can perform an arbitrary nonlinear transformation $\phi(x)$ of the inputs x and then linearly combine the components of this transformation.
- $\phi : \mathbb{R}^D \to \mathbb{R}^K$ is called the basis function

Basis Functions

Some examples of basis functions:

- Polynomial basis: $\phi(x) = \{1, x, x^2, x^3, \dots\}$

Basis Functions

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- Polynomial basis: $\phi(x) = \{1, x, x^2, x^3, \dots\}$
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  $\phi(x) = \{1, \exp(-\frac{(x-\mu_1)^2}{2\sigma^2}), \exp(-\frac{(x-\mu_2)^2}{2\sigma^2}), \dots\}$

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  $\phi(x) = \{1, \exp(-\frac{(x-\mu_1)^2}{2\sigma^2}), \exp(-\frac{(x-\mu_2)^2}{2\sigma^2}), \dots\}$
- Sigmoid basis: $\phi(x) = \{1, \sigma(x - \mu_1), \sigma(x - \mu_2), \dots\}$
  where $\sigma(x) = \frac{1}{1+e^{-x}}$

Linear Combination of Vectors

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$$\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \alpha_3 \mathbf{v}_3 + \cdots + \alpha_i \mathbf{v}_i$$

where $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_i \in \mathbb{R}$

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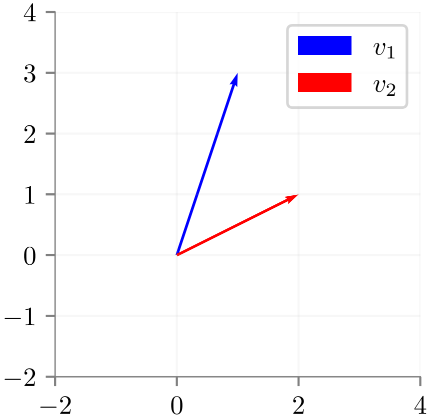
It is the set of all vectors that can be generated by linear combinations of $v_1, v_2, \ldots, v_i$.
If we stack the vectors $v_1, v_2, \ldots, v_i$ as columns of a matrix V, then the span of $v_1, v_2, \ldots, v_i$ is given as $V\alpha$ where $\alpha \in \mathbb{R}^i$

Example

Find the span of $\left(\begin{bmatrix}1\\3\end{bmatrix}, \begin{bmatrix}2\\1\end{bmatrix}\right)$



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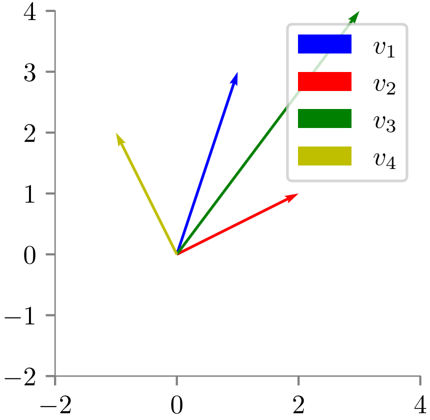
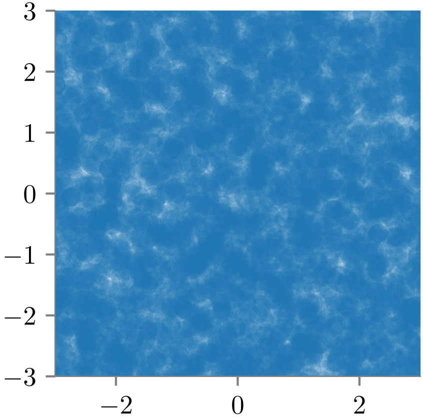


We have $v_3 = v_1 + v_2$
We have $v_4 = v_1 - v_2$

Example

Simulating the above example in python using different values of α_1 and α_2



Span$((v_1, v_2)) \in \mathcal{R}^2$

Example

Find the span of $\left(\begin{bmatrix}1\\2\end{bmatrix}, \begin{bmatrix}2\\4\end{bmatrix}\right)$

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Find the span of ($\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 2 \\ 4 \end{bmatrix}$)

Can we obtain a point (x, y) s.t. x = 3y?

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No

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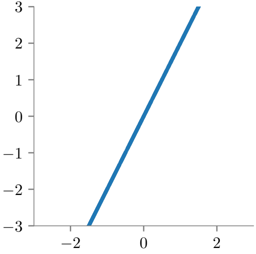
Span of the above set is along the line y = 2x



Example

Find the span of $\left(\begin{bmatrix}1\\1\\1\end{bmatrix}, \begin{bmatrix}2\\-2\\2\end{bmatrix}\right)$

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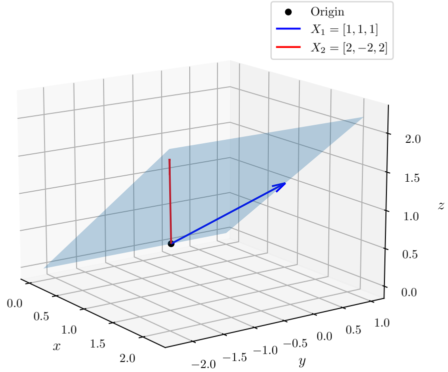

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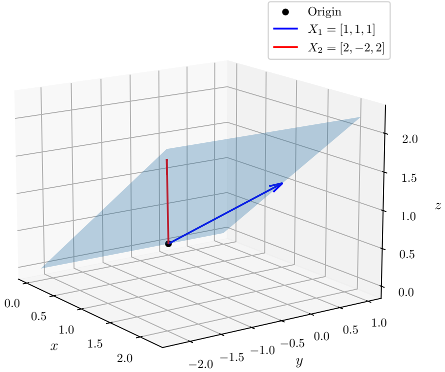

The span is the plane $z = x$ or $x_3 = x_1$

Geometric Interpretation

Consider $\mathbf{X}$ and $\mathbf{y}$ as follows.

$$\mathbf{X} = \begin{pmatrix} 1 & 2 \\ 1 & -2 \\ 1 & 2 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 8.8957 \\ 0.6130 \\ 1.7761 \end{pmatrix}$$

- We are trying to learn $\boldsymbol{\theta}$ for $\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$ such that $||\mathbf{y} - \hat{\mathbf{y}}||_2$ is minimised

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- Consider the two columns of $\mathbf{X}$. Can we write $\mathbf{X}\boldsymbol{\theta}$ as the span of ($\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ -2 \\ 2 \end{bmatrix}$)?
- We wish to find $\hat{\mathbf{y}}$ such that

$$\underset{\hat{\mathbf{y}} \in SPAN\{\bar{x_1}, \bar{x_2}, \ldots, \bar{x_D}\}}{\arg\min} ||\mathbf{y} - \hat{\mathbf{y}}||_2$$

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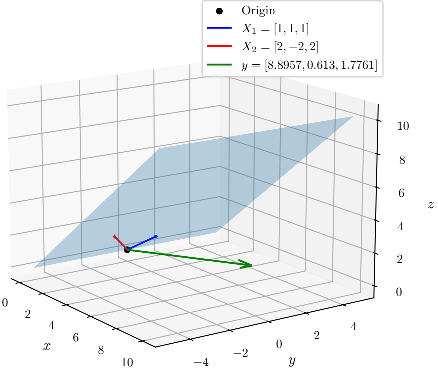

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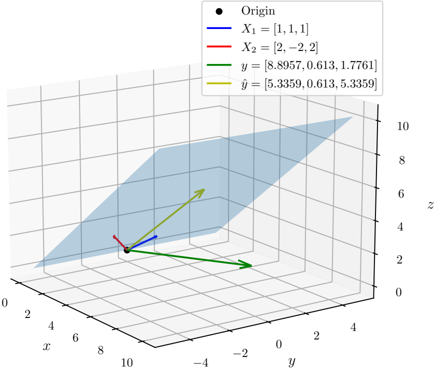

- We seek a $\hat{\mathbf{y}}$ in the span of the columns of $\mathbf{X}$ such that it is closest to $\mathbf{y}$

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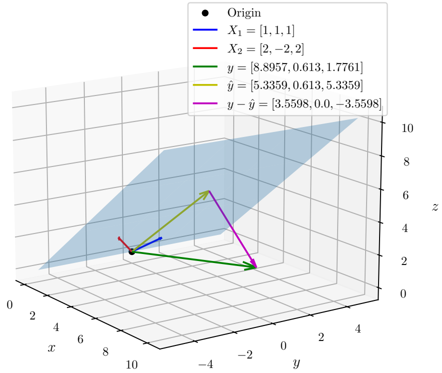

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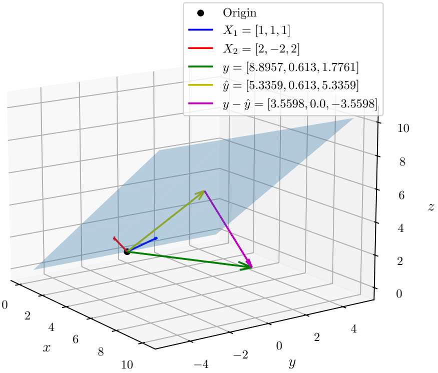

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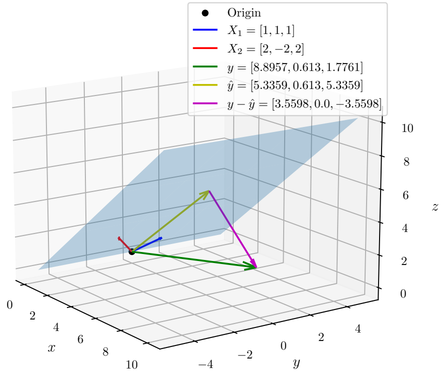

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- $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = 0$
- $\mathbf{X}^\top\mathbf{y} = \mathbf{X}^\top\mathbf{X}\boldsymbol{\theta}$ or $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$

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- This prevents coefficients from becoming too large

Ridge Regression (L2 Regularization)

Objective Function:

$$J(\boldsymbol{\theta}) = \text{MSE} + \lambda \sum_{j=1}^{n} \theta_j^2$$

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- Note: $(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})$ is always invertible for $\lambda > 0$

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$$J(\boldsymbol{\theta}) = \frac{1}{2m}\sum_{i=1}^{m}(h_{\boldsymbol{\theta}(\mathbf{x}^{(i)})-y^{(i)})^2+\lambda\sum_{j=1}^{n}|\theta_j|}$$

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- **Use Case**: When you suspect many features are irrelevant

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- **Elastic Net**: Combines both penalties

$$J(\boldsymbol{\theta}) = \text{MSE} + \lambda_1 \sum |\theta_j| + \lambda_2 \sum \theta_j^2$$

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- **Critical Insight**: λ controls bias-variance tradeoff

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$$X = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 3 & 6 \end{bmatrix} \tag{1}$$

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The matrix X is not full rank.

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How to tackle it?

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- Avoid dummy variable trap

Dummy variables

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Can we use the direct encoding?
Then this implies that S$>$W$>$E$>$N

Dummy Variables

N-1 Variable encoding

	Is it N?	Is it E?	Is it W?
N	1	0	0
E	0	1	0
W	0	0	1
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Dummy Variables

N Variable encoding

	Is it N?	Is it E?	Is it W?	Is it S?
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Is it S = 1 - (Is it N + Is it W + Is it E)

Binary Encoding

N	00
E	01
W	10
S	11

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W and S are related by one bit.

Binary Encoding

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W and S are related by one bit.
This introduces dependencies between them, and this can cause confusion in classifiers.

Interpreting Dummy variables

Gender	height
F	...
F	...
F	...
M	...
M	...

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Gender	height
F	...
F	...
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Encoding

Interpreting Dummy variables

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Encoding

Is Female	height
1	...
1	...
1	...
0	...
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Interpreting Dummy Variables

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Is Female	height
1	5
1	5.2
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0	5.8
0	6

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$height_i = \theta_0 + \theta_1 * (\text{Is Female}) + \epsilon_i$

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We get θ_0 = 5.9 and θ_1 = -0.7
θ_0 = Avg height of Male = 5.9

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1	5
1	5.2
1	5.4
0	5.8
0	6

$height_i = \theta_0 + \theta_1 * (\text{Is Female}) + \epsilon_i$

We get $\theta_0 = 5.9$ and $\theta_1 = -0.7$
θ_0 = Avg height of Male = 5.9
$\theta_0 + \theta_1$ is chosen based (equal to) on 5, 5.2, 5.4 (for three records).

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Now, θ_0 can be interpreted as average person height. θ_1 as the amount that female height is above average and male height is below average.

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